26 June 2001

John DaMassa
Planning & Technical Support Division
California Air Resources Board
P.O. Box 2815
Sacramento, CA 95812

Dear John,

Attached please find my detailed review comments on the modeling protocol document for southern California that you provided. A summary of my major comments is provided below. This review was completed under interagency agreement 98-004 between the University of California and the California Air Resources Board.

The protocol document is an important communication mechanism within the modeling team, and with external stakeholders and technical experts. A clearer statement of objectives for the modeling study is needed at the beginning of the protocol document.

The most adverse meteorological conditions leading to high ozone levels were not seen during SCOS97; it is appropriate to consider other more severely polluted episodes as part of an attainment demonstration for southern California.

Major reductions in air pollutant emissions and ozone levels were observed between 1987 and 1997 in southern California. I recommend updated emission estimates be developed for a summer 1987 (SCAQS) episode, and modeling be conducted of the changes in ozone that took place between 1987 and 1997.

Numerical guidelines for model performance, measured in terms of normalized bias and gross error of the ozone predictions, have been overemphasized. Decisions about which models and input data are "best" and "state-of-science" should not focus only on agreement between observed and predicted ozone levels. Many compensating errors may be present in model algorithms and inputs, and better models may reveal problems that were previously hidden.

Attempts should be made to understand and reconcile potentially large and influential uncertainties in off-road diesel engine NO_x emissions.

This modeling study continues California's tradition of being at the leading edge of developing model inputs and using photochemical models to develop air quality management plans. I am very impressed by all the progress that has been made on many fronts since SCAQS in 1987. I encourage you to publish in peer-reviewed journals some of the insights that will surely be gained in this effort.

I hope my comments are constructive and will be helpful to you as the modeling effort continues. Please call me at (510) 643-9168 if you have any questions.

Sincerely,

Robert Harley
Associate Professor

Attachment: detailed peer review comments.

Review of

Modeling Protocol for Regional 1-Hour and 8-Hour Ozone Modeling in Southern California for the 2003 State Implementation Plans

Inter-Agency Agreement 98-004

Prepared for

Planning & Technical Support Division
California Air Resources Board
P.O. Box 2815
Sacramento, CA 95812

Prepared by

Robert Harley, Associate Professor
Department of Civil and Environmental Engineering
University of California
Berkeley, CA 94720-1710

June 26, 2001

Introduction

The subject of this peer review is a photochemical modeling protocol document for southern California, draft #3 dated September 18, 2000. In addition to reviewing the protocol document, the review process included a daylong meeting with ARB and SCAQMD staff in Sacramento, and a follow-up conference call on mobile source emissions issues. Although other University of California scientists are expected to be involved in reviewing the modeling protocol, the review comments presented here were developed without consulting other reviewers. This approach was desired by ARB staff to provide a greater range of peer review comments, and more opportunity for staff to interact with individual reviewers.

According to DaMassa (1992), the modeling protocol process and document are essential features of a modeling study, laying the foundation for the technical work that will follow, and providing an early and appropriate opportunity for external review before the work is conducted.

Background and Objectives of Modeling Study

Major field studies of photochemical air pollution were conducted in southern California in summer 1987 (Southern California Air Quality Study or SCAQS) and summer 1997 (Southern California Ozone Study, SCOS97). The protocol document provides an appropriate overview of SCOS97, including objectives and scope of the field study. *The objectives of the proposed photochemical modeling work should be listed and described more clearly at the beginning of the protocol document*. For example, modeling objectives could include some or all of the following: (1) model evaluation for recent (1997-98) air pollution episodes in southern California, (2) assessment of inter-basin transport of ozone and precursors, (3) selection of state-of-science model(s) to use in future air quality planning efforts, (4) assessment of changes in precursor emissions and ozone levels in southern California between 1987 and 1997, (5) attainment demonstration for ozone in the South Coast Air Basin and other neighboring areas, (6) study of weekday-weekend differences in ambient ozone levels and precursor emissions. There may be other objectives as well.

Modeling Domain

The proposed geographic extent of the air quality modeling region is presented in Figure 1 of the protocol document. This domain is large, extending well beyond the urbanized areas of the South Coast Air Basin. Such a domain is necessary for photochemical modeling if inter-basin transport issues are to be assessed.

On page 3, the statement that “terrain elevations in Southern California often exceed 2000 m AGL” is incorrect, because local terrain height is always defined to be 0 m above ground level (AGL). I think the authors mean 2000 m MSL (i.e., above mean sea level).

Choices of different locations for boundaries of the modeling domain will not necessarily minimize the influence of boundary conditions on simulation results… the numerical values of the boundary conditions used in the modeling are also important.

Episode Selection

Concerns about past regulatory photochemical modeling studies in southern California included a lack of weekend episodes (when ozone concentrations tend to be higher on average), and dropping a severe episode from summer 1985 from the attainment demonstration in the 1997 AQMP.

Six different air pollution episodes from 1997 and 1998 are proposed for further consideration in Table 1. The list includes a weekend episode (26-29 September 1997, a Friday through Monday), and several other episodes that include one or more weekend days. Unfortunately, SCOS97 failed to capture any high-ozone episodes describing photochemical air quality in the basin under the most adverse meteorological conditions. *It would be helpful to include in the protocol document a review of the El Niño effect,* and discuss how it may have affected precipitation, cloudiness, and temperature in southern California in 1997 and 1998.

Whereas the episodes from 1997 have an extensive supporting aerometric database from SCOS97, the 14-19 July 1998 episode listed in Table 1 was more severe than any of the others listed. I*t would be appropriate to consider the 14-19 July 1998 episode as part of a determination of the emission-carrying capacity of the South Coast Air Basin and neighboring areas.*

The summer 1987 SCAQS air pollution episodes remain of historical interest. *Inclusion of one SCAQS episode (e.g., 23-25 June 1987) should be considered*, as part of an assessment of how emissions and air quality have changed in southern California over the intervening decade between 1987 and 1997.

Air Quality Model Selection

The modeling protocol mentions concerns that the current regulatory air quality model (UAM-IV) has limitations that make it unsuitable for regional-scale photochemical modeling. A variety of newer models including CALGRID, CAMx, CMAQ, SAQM, UAM-FCM, and UAM-V are mentioned as candidate models for further study.

I recommend against selecting or deselecting models based solely on the level of agreement between observed and predicted ozone levels. The possibilities for compensating errors in model inputs and model algorithms are legion. A better model may appear to be inferior in terms of ozone performance, only because an improved description of one or more processes may reveal other problems that were previously hidden. Detailed review of model components such as advection algorithm, chemical mechanism, dry deposition module, numerical integration scheme, documentation, ease

of input data preparation and output postprocessing, etc. should all be considered as factors to decide which models are to be recommended for use.

At the bottom of page 9, the text states that ARB and SCAQMD staff have agreed to begin testing UAM-V, among other models, for the SCOS97 domain. This seems inconsistent with text immediately above stating that the present non-public domain status of UAM-V precludes regulatory usage.

I am concerned about the multiplicity of air quality model/air pollution episode combinations. There are 6 different air quality models, and 6 or more air pollution episodes proposed for further study. *Applying all of the proposed air quality models to all of the air pollution episodes is unlikely to be a productive use of staff time*. A strategy for deciding on which air quality model(s) will be used should be described, and this strategy should be executed early so the multiplier effect doesn't overwhelm the ability to gain and communicate insights from the modeling effort.

Chemical Mechanism

In the past, air quality models contained a "hardwired" chemical mechanism that was an integral part of the model and could not easily be changed. More recently, air quality models have evolved so that the chemical mechanism can often be described as a model input. The Carbon Bond-IV mechanism (Gery et al., 1989) lacks options for detailed resolution of VOC chemistry, and is no longer "state-of-the-science" in my opinion.

VOC lumping strategies should be discussed in the protocol document. It may be worthwhile to include MTBE and ethanol as explicit species in the chemical mechanism, since major changes in emissions of these species have occurred or will occur in southern California due to gasoline reformulation. It may also be worthwhile to include methylbutenol (MBO) as a separate, explicit model species in the mechanism, since the biogenic emission inventory now includes this species. In general, biogenic and anthropogenic VOC should not be lumped together, since their spatial and temporal patterns differ, and no single characterization of lumped species properties will apply throughout the modeling domain if biogenic and anthropogenic VOC are combined. These changes should help stabilize the mix of VOC assigned to each lumped species, and hopefully minimize changes in lumped species properties over time.

In summary, *more detailed discussion of chemical mechanisms and VOC lumping should be added to the protocol document.*

Horizontal and Vertical Grid Resolution

The horizontal grid resolution is proposed to be 5 km, which is consistent with past practice. The extent of the modeling domain is larger now, so there will be more grid squares. MM5 and CALMET provide wind fields and other meteorological inputs on different grid systems – Lambert Conformal for MM5 and a UTM-based grid system for CALMET, so two different sets of gridded emission estimates will be needed.

To facilitate inter-comparison of model predictions, *it is recommended that the same or similar vertical cell heights be used where possible*, especially for the lowest layer near the earth's surface. Large differences may arise in primary pollutant concentrations at night if pollutants remain trapped within the ground-level cell. Tables 2 and 3 currently indicate different ground-level cell heights of 61 and 20 meters, respectively. In Table 2, it is not clear why the air quality model extends all the way to the top of troposphere. Is it possible for significant exchange to occur between the uppermost cells and lower layers on the time-scale that air masses remain within the modeling domain? In Table 3, the vertical heights for cells 4 and 5 are incorrect.

Meteorological Inputs

The protocol document discusses three different types of models that can be used to generate the meteorological inputs needed for air quality modeling. The objective and diagnostic models rely on interpolation of observations, whereas prognostic models solve coupled conservation equations for fluid mass, momentum, energy, and water content. A procedure known as four-dimensional data assimilation (FDDA) allows the predictions of prognostic models to be nudged towards observations when and where they are available. A more detailed review is provided by Seaman (2000).

The southern California modeling domain includes complex topography, with mountains as high as 3000 meters or more above sea level, with associated upslope and downslope flows that are difficult to model. Meteorological observations are sparse within mountainous and unpopulated desert areas. Inter-basin transport sometimes occurs through mountain passes (e.g. Banning Pass connects the South Coast and Salton Sea air basins). Development of accurate meteorological fields for this domain is a challenging task, regardless of the modeling approach that is used. The larger modeling domain and the desire to assess inter-basin transport place greater demands on the met modeling, especially with respect to flow over complex terrain.

The use of radar wind profilers has greatly expanded the frequency of wind observations aloft, though relative to SCAQS we may have lost ground in obtaining temperature and humidity data aloft (soundings conducted using balloons typically provide vertical temperature and humidity profiles that are useful in locating the inversion layer). Further consideration of the adequacy of the observational database (wind, temperature, and humidity) throughout the full horizontal and vertical extent of the modeling domain is needed before objective/diagnostic modeling approaches can be considered as a source of met inputs for the air quality models.

On page 16, there is a vague statement that met-fields "will be evaluated to determine which is most suitable for air quality modeling." The text beginning on page 17 (validation and technical review) provides more specific methods for evaluation. The ability to simulate tracer release experiments accurately could be helpful in making decisions about which met fields to use in air quality modeling. *Decisions about which met-fields will be used should not be made by looking for best agreement with observed*

ozone levels, because of the possibilities of compensating errors in other model inputs and algorithms, as discussed above.

In the past, separate met modeling approaches have been used for individual episodes within the scope of a single planning study. This situation should be avoided in the future. However, it may be necessary to use different met modeling procedures for the 14-19 July 1998 episode, since not all of the met observations from SCOS97 continued in the following summer.

Emission Inventory

Assembling accurate emission estimates throughout the large southern California modeling domain will be a very challenging task. There are many different agencies involved in the effort, including numerous local air pollution control and transportation/ land use planning agencies, Air Resources Board staff in El Monte and Sacramento, and various contractors.

Point and Area Sources

Point source emission estimates are available for 1996 and are being compiled for 1997. An emission forecasting system (Johnson and Lakhanpal) will be used where point source estimates are not available for the year and sub-region in question. The situation is similar for area sources. Updating the inventory is difficult because of the need to reconcile point and area source estimates to prevent double-counting (Bickett). Furthermore, emission estimates must be collected from local air districts and ARB staff.

Mobile Sources

Concerns about past photochemical modeling studies in southern California focused on questions of negative bias in the hydrocarbon emission inventory, representation of weekday vs. weekend changes in motor vehicle activity and emissions, and representation of the different spatial and temporal patterns appropriate for heavy-duty diesel trucks. Major efforts have been made by ARB staff over the last 10 years to address these and other concerns. New models (EMFAC 2000 and OFFROAD) have been developed to estimate mobile source emissions, and hydrocarbon emission estimates have increased compared to earlier versions of EMFAC. Emission sources such as leaking liquid gasoline from poorly-maintained vehicles have been recognized and are now estimated in the emission inventory. A freight-based travel demand model and weigh-in-motion traffic counters are being used to improve the representation of diesel truck travel and emissions in southern California.

ARB staff have used a variety of methods to assess estimates of mobile source emissions (ARB, 2001). These verification methods include comparisons with Van Nuys tunnel results from 1987 and 1995, comparison with remote sensing-based estimates of CO and HC emissions obtained during SCOS97 (Singer et al., 2000), and comparisons of fuel consumption estimates from the models with statewide fuel tax returns. It is surprising

that EMFAC 2000 is predicting no change in diesel fuel consumption in the state through the 1990s.

The Van Nuys tunnel provided unique and early on-road measurements of vehicle emissions from 1987, but this tunnel is short (220 meters) and uncertainties in measured emission factors tend to be large. For more recent years (1995 and 1996), measurements by Gertler et al. (1999) at the longer Sepulveda Tunnel in southern California may provide more useful points of reference for comparison with EMFAC model predictions.

Other assessments that should be reviewed address questions such as the relative importance of tailpipe vs. evaporative sources of HC emissions (Pierson et al., 1999), gasoline vs. diesel engine contributions to on-road vehicle NO_x emissions (Kirchstetter et al., 1999; Sawyer et al., 2000), the importance of off-road diesel engines as a source of NO_x emissions (Kean et al., 2000), and the contributions of cold start vs. stabilized operating conditions to total exhaust emissions (Singer et al., 1999).

A potentially large and influential uncertainty is off-road diesel engine activity and associated NO_x emissions. Kean et al. (2000) used fuel sales surveys conducted by the U.S. Energy Information Administration (EIA) to estimate off-road diesel engine activity. In contrast, the OFFROAD model relies on estimates of number of engines, hours of use, and load factor, broken down by horsepower rating and end-use application of the engines. Using statewide data for California from 1996, off-road diesel NO_x emissions in the construction and agricultural sectors are estimated to be 98 and 37 tons per day, respectively (see Kean et al. 2000 for supporting data). California's OFFROAD model estimates for calendar year 2000 predict NO_x emissions that are ~3 times higher. Differences in activity estimates were identified by Kean et al. as a source of uncertainty. *Uncertainties in the estimates of off-road diesel engine emissions are large enough to recommend further in-depth study, and consideration of alternate emission scenarios in the photochemical modeling if the estimates cannot be reconciled.*

Major efforts to control mobile source emissions were made through the 1990s, including more effective and durable control technologies installed on new vehicles, reformulated fuels, and enhanced inspection and maintenance. A dramatic decrease in photochemical air pollution in southern California has been observed over the same time period. *Historical emission estimates for 1987 should be developed to support modeling of the changes in ozone levels that have occurred between SCAQS in 1987 and SCOS97.*

Day-Specific Emissions

Changes in environmental conditions (mainly temperature) and day of week (especially weekday vs. weekend) lead to changes in air pollution emissions. Unusual events such as wildfires and shutdowns at major point sources can also affect emissions and air quality. For aircraft, it would be useful to develop day-of-week estimates (typical weekday, Friday, Saturday, and Sunday). The differences from day to day should be assessed, to provide guidance as to whether data should be collected for each specific modeling episode, or whether generic day-of-week estimates can be used.

Natural Emissions

Emissions of isoprene, monoterpenes and methylbutenol will be estimated for the modeling region using a biogenic emission inventory system, BEIGIS. *As anthropogenic emissions decline, the relative importance of biogenic emissions is likely to increase.* Compared to estimates used in past modeling, updates to the biogenic emission inventory include new plant species data as a function of land use, updated emission factors and dependence on environmental conditions, and inclusion of a new species (methylbutenol) emitted by pine trees.

Organic Gas Speciation

Reformulation of gasoline in California that took effect in 1995-96 has led to major changes in VOC speciation from mobile sources. New speciation profiles are therefore needed to represent conditions in 1997/1998.

Northern Mexico Inventory

It is not clear whether the modeling domain shown in Figure 1 includes enough of northern Mexico to make a meaningful assessment of air pollution transport between Mexico and southern California. How will the boundary condition at the southern edge of the modeling domain be specified?

Initial and Boundary Conditions

The modeling region is larger than used in past studies, so the "spin-up" time required to remove the influence of uncertainties in initial conditions may be longer now. *It is recommended that simulation spin-up should begin during the mid-afternoon rather than at midnight*, so that surface observations used to specify IC are more likely to represent pollutant concentrations in the first ~500 meters accurately. Using observations from midnight to initialize the model is likely to represent concentrations in only the first ~50 meters of the modeling domain.

As noted above, *prescribing a large modeling region does not guarantee the influence of boundary conditions is minor*. The numerical values used for the boundary conditions are also important. The amounts of formaldehyde, ozone, PAN, and NO_x at the boundaries may be particularly influential. The rationale and methodology for altering BCs for modeling future-year scenarios should be presented. Sensitivity studies are needed to assess the importance of BCs, as described on p. 31 of the protocol document.

Model Performance Evaluation

Numerical guidelines for model performance, measured in terms of normalized bias and gross error (DaMassa, 1992) are a useful point of reference, but *have been over-*

emphasized, and may lead to bad decisions about the most appropriate air quality models and input data to be used.

In addition to evaluating model predictions for ozone using graphical and statistical techniques, and investigating model responses in a series of diagnostic simulations, I *recommend evaluations of model predictions for total NMOC, nitric oxide* (NO is measured directly by chemiluminescent analyzers, CLA), *and NO_y* (meaningful only at sites with externally mounted converters on the CLA). Comparing the distribution of total NO_y among NO, NO_2, PAN, PPN, HNO_3, alkyl nitrates, etc. would be another useful test of model predictions vs. observations, though there are probably only a few research sites where this comparison of NO_y speciation is possible. Evaluation of chain-initiating (HCHO, HONO) and chain-terminating (H_2O_2, CH_3OOH, and HNO_3) species predictions may also be possible at a few sites.

Use of the Modeling Results

Applications for the modeling results include estimation of the carrying capacity for ozone precursors, demonstration of attainment of air quality standards, and assessment of inter-basin transport. *A useful test case for evaluating the relative response factor (RRF) would be to look at changes that occurred in observed and predicted air quality in southern California between 1987 SCAQS and SCOS97*.

The protocol document should clarify the rationale for looking at 1-hour peak ozone concentrations, now that EPA's 8-hour ozone standard has been sustained in court and the Federal 1-hour ozone standard has been abolished.

Deliverables

The protocol document envisions a large effort involving many people and a year or more of effort. The regulatory mission of the agencies involved means that a top priority must be development of state implementation plans for attainment of air quality standards. If time and resources permit, *it would also be desirable to publish selected aspects of this modeling study in the peer-reviewed literature*. This would provide appropriate recognition and visibility for staff efforts, and a means for continuing professional development. Rather than a single omnibus paper, more focused reports could be written with individual staff members taking the lead in presenting noteworthy findings.

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